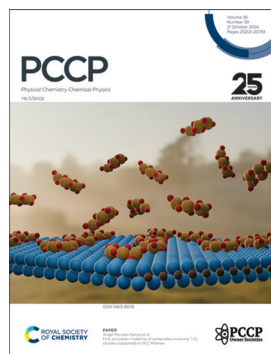


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See Ángel Morales-García *et al.*, pp. 25319–25328. Image reproduced by permission of Ángel Morales-García from *Phys. Chem. Chem. Phys.*, 2024, 26, 25319.



### Inside cover

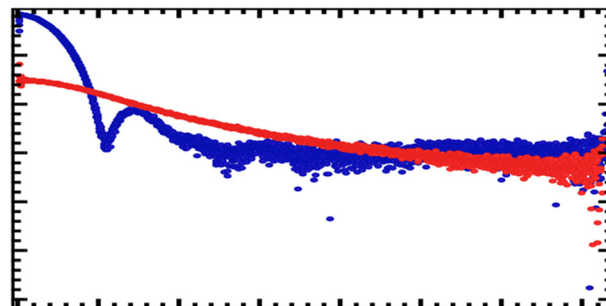
See Zhen Zhao, Bo Li *et al.*, pp. 25329–25340. Image reproduced by permission of Bo Li from *Phys. Chem. Chem. Phys.*, 2024, 26, 25329.

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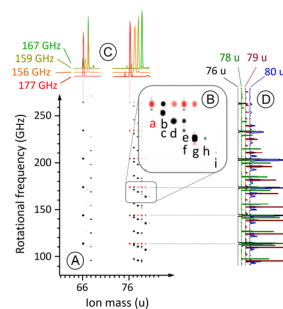
Ahmed S. A. Mohammed, Dmytro Soloviov and Cy M. Jeffries\*



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Thomas Schultz



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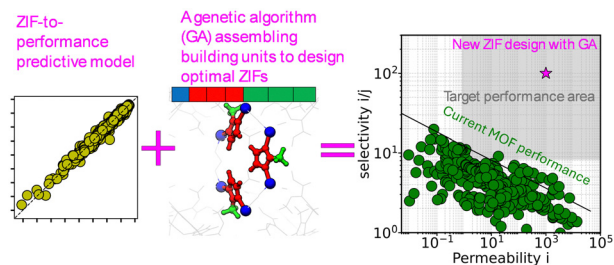


## COMMUNICATION

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Panagiotis Krokidas,\* Michael Kainourgiakis, Theodore Steriotis and George Giannakopoulos

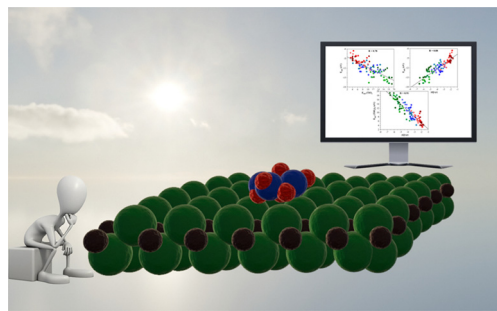


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**First principles modeling of composites involving  $\text{TiO}_2$  clusters supported on  $\text{M}_2\text{C}$  MXenes**

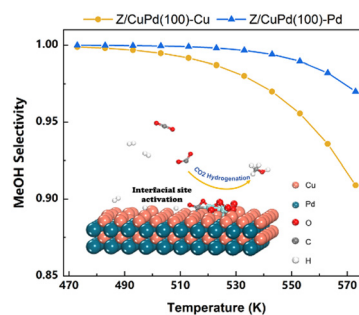
Masoomah Keyhanian, Néstor García-Romeral, Ángel Morales-García,\* Francesc Viñes and Francesc Illas



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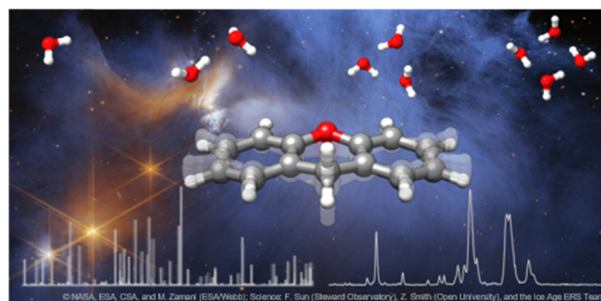
Bin Qin, XiaoYing Sun, Jianzhuo Lu, Zhen Zhao\* and Bo Li\*



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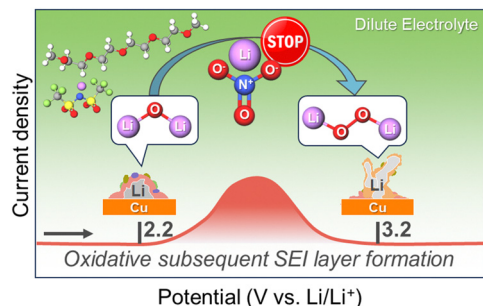
**Probing the structure and dynamics of the heterocyclic PAH xanthene and its water complexes with infrared and microwave spectroscopy**

Donatella Loru,\* Wenhao Sun, Hugo Nootebos, Amanda L. Steber, Piero Ferrari and Melanie Schnell\*



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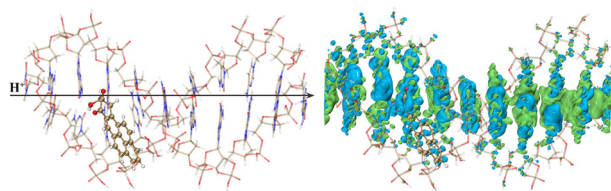
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### Revealing the enhancement of Li plating/stripping efficiency in TEGDME-based low-concentration electrolytes for anode-free lithium metal batteries

Yushen Wang and Hidenori Noguchi\*

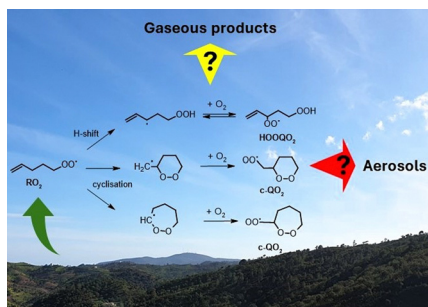
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### Effects of BPQ binding on the nonadiabatic dynamics of excited electrons in poly(dG)–poly(dC) DNA under proton irradiation

Zhihua Hu, Zun-Yi Deng and Hong-Jian Feng\*

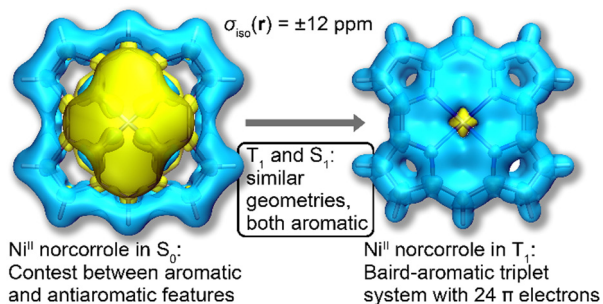
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### H-shift and cyclization reactions in unsaturated alkylperoxy radicals near room temperature: propagating or terminating autoxidation?

Barbara Nozière\* and Luc Vereecken\*

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### Excited-state aromaticity reversals in norcorrole

Peter B. Karadakov\* and Edward Cummings

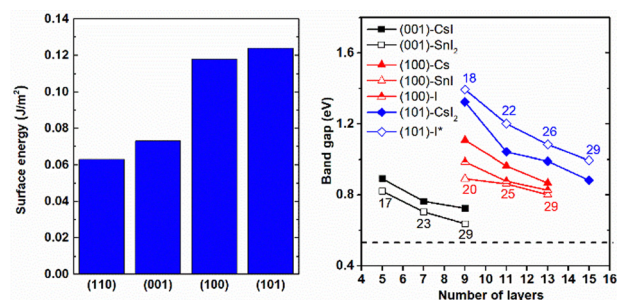


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First-principles study of the surface energies and electronic structures of  $\gamma$ -CsSnI<sub>3</sub> surfaces

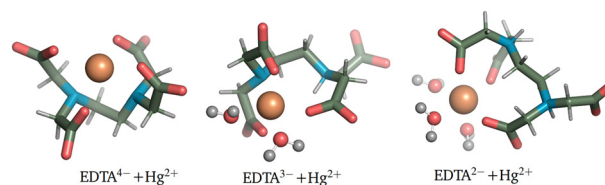
Tong Zhou, Yan-Jin Chen, Chunju Hou\* and Yi Yang\*



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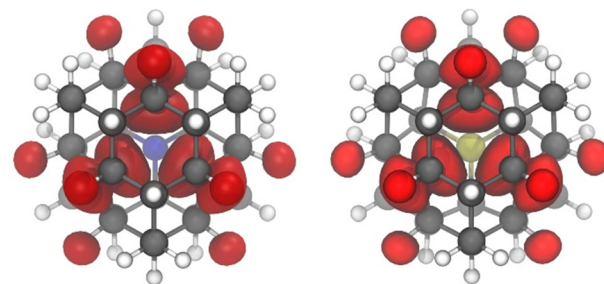
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Heteroatom-vacancy centres in molecular nanodiamonds: a computational study of organic molecules possessing triplet ground states through  $\sigma$ -overlap

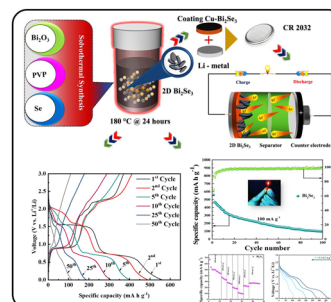
Colette Maya Macarios, Jiří Pittner, Viki Kumar Prasad and Ulrich Fekl\*



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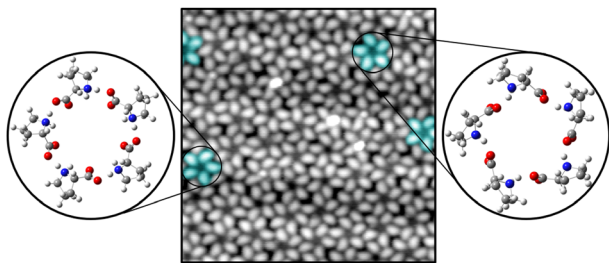
Exploring the electrochemical performance of layered Bi<sub>2</sub>Se<sub>3</sub> hexagonal platelets as the anode material for lithium-ion batteries

Shaik M. Abzal, Sumit Khatua, Kurapati Kalyan, SaiLakshmi Janga, Rajkumar Patel\*, L. N. Patro\* and Jatis Kumar Dash\*



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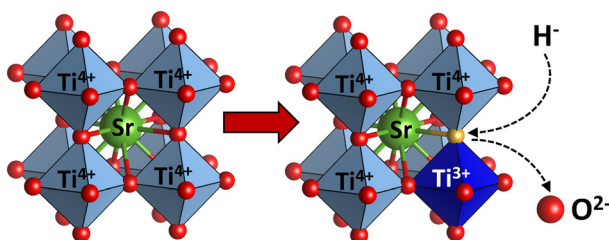
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### Enantiopure molecules form apparently racemic monolayers of chiral cyclic pentamers

Benjamin R. Heiner, Kaitlyn M. Handy, Angela M. Devlin, Jewel L. Soucek, Alexander M. Pittsford, David A. Turner, Jacob P. Petersen, Allen G. Oliver, Steven A. Corcelli and S. Alex Kandel\*

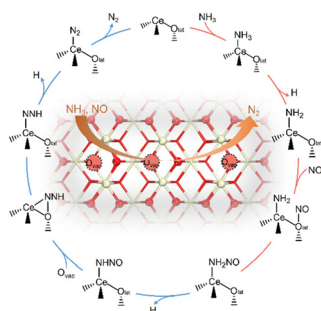
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### The spectroscopy of hydride in single crystals of SrTiO<sub>3</sub> perovskite

William R. Palfey,\* Son-Jong Hwang, William A. Goddard III and George R. Rossman

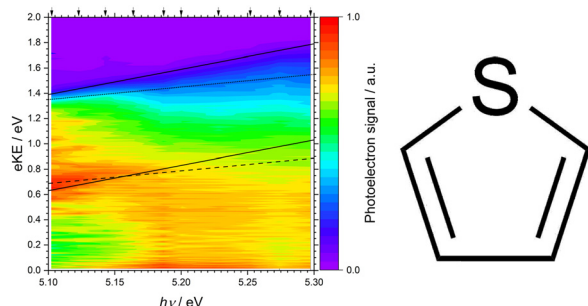
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### Mechanistic insights into NH<sub>3</sub>-assisted selective reduction of NO on CeO<sub>2</sub>: a first-principles microkinetic study on selectivity and activity

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### A multiphoton ionisation photoelectron imaging study of thiophene

Joseph J. Broughton, Sarbani Patra, Michael A. Parkes, Graham A. Worth and Helen H. Fielding\*

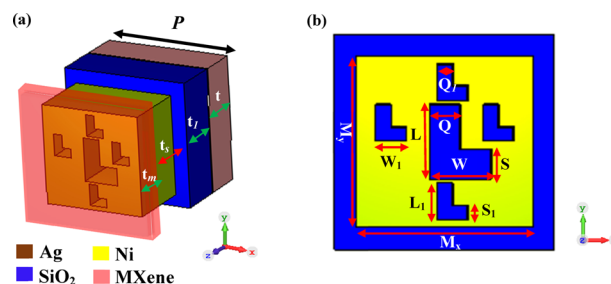


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# A high-performance ultra-wideband metasurface absorber and thermal emitter for solar energy harvesting and thermal applications

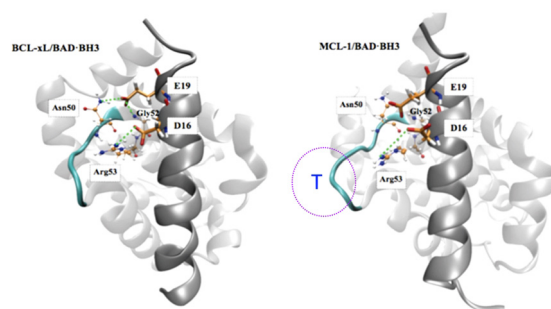
Ammar Armghan, Meshari Alsharari, Muhammad Abuzar Baqir, Muhammad Saqlain\* and Khaled Aliqab



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# Theoretical study on the selective binding of BH3-only protein BAD to anti-apoptotic protein BCL-xL instead of MCL-1

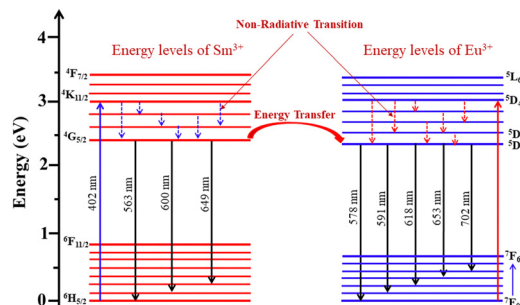
Panpan Wang, Jinglan Cui,\* Guojie Cheng and Dawei Zhang\*



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# $\text{Eu}^{3+}$ singly-doped and $\text{Eu}^{3+}/\text{Sm}^{3+}$ co-doped ZnS quantum dots: structure, optical properties and energy transfer

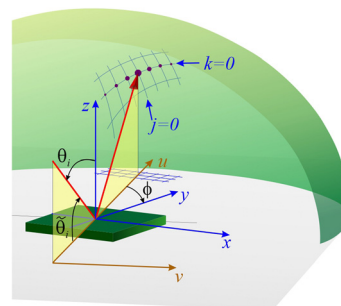
N. T. M. Thuy, T. T. T. Huong, N. T. Hien, N. T. Luyen, N. T. Kien, N. T. K. Van, P. M. Tan, N. D. Vinh, T. Ngoc and N. X. Ca\*



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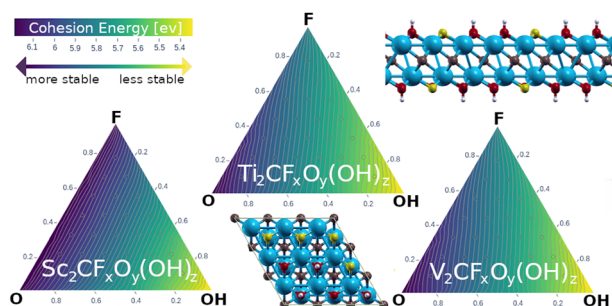
# Grazing incidence fast atom diffraction: general considerations, semiclassical perturbation theory and experimental implications

E. Pollak, P. Roncin, W. Allison and S. Miret-Artés\*



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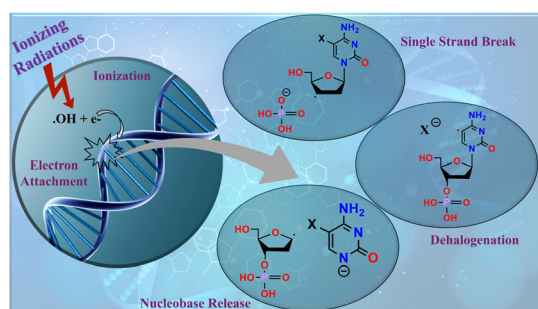
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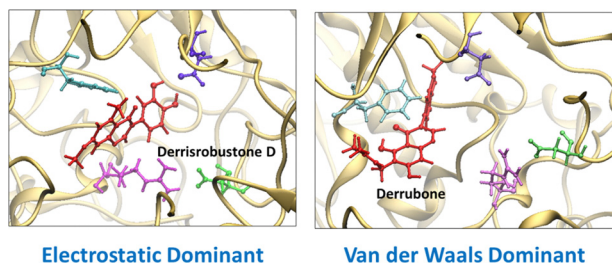
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### Dissociative electron attachment to halogenated nucleotides: a quest for better radiosensitizers

Shubham Kumar and Manabendra Sarma\*

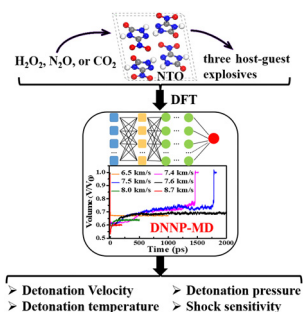
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### The potentiality of isoflavones from *Derris robusta* (DC.) Benth. against $\alpha$ -glucosidase

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### Detonation performance and shock sensitivity of energetic material NTO with embedded small molecules: a deep neural network potential accelerated molecular dynamics study

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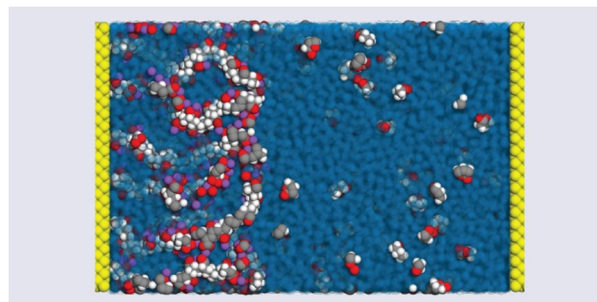


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### All-atom molecular dynamics simulations showing the dynamics of small organic molecules in water-solvated polyelectrolyte brush layers

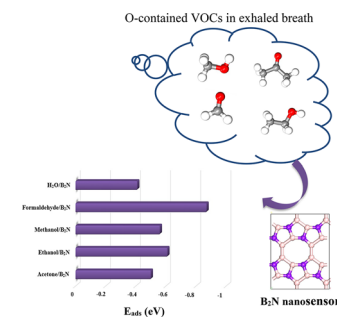
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### Exploring the adsorption behavior of O-containing VOCs in human breath on a B<sub>2</sub>N monolayer using DFT simulations

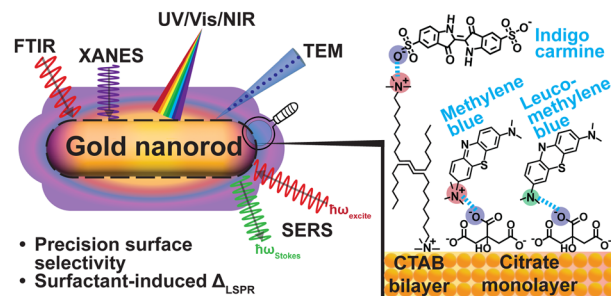
Rezvan Rahimi\* and Mohammad Solimannejad\*



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### Targeted synthesis of gold nanorods and characterization of their tailored surface properties using optical and X-ray spectroscopy

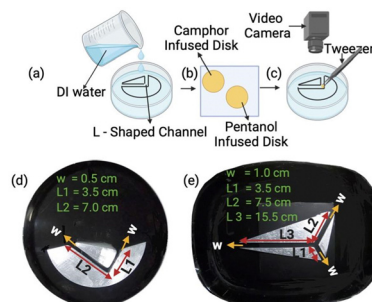
David G. Schauer, Jona Bredehoeft, Umar Yunusa, Ajith Pattammattel, Hans Jakob Wörner and Emily A. Sprague-Klein\*



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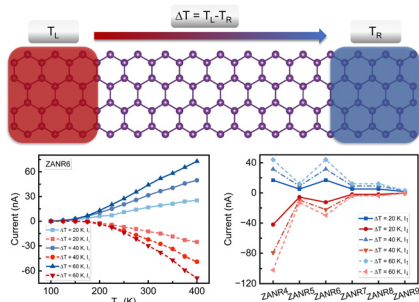
### Surface tension gradient invoked path selection

Anjuman Ara Khatun,\* Aarsh Chotalia, Kalpita Das, Shiva Dixit and P. Parmananda



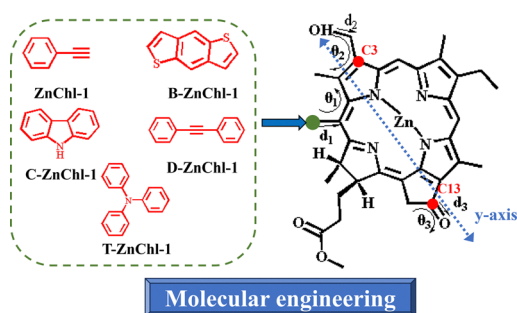
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**Spin-dependent Seebeck effect in zigzag-edge antimonene nanoribbons**

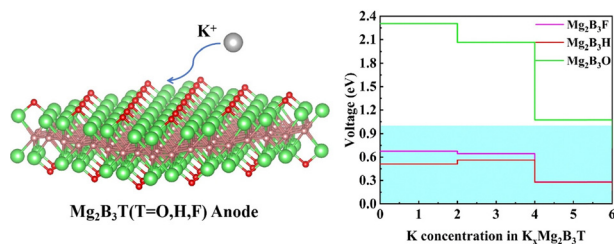
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**Molecular engineering and structure–property relationship based on D–A chlorophyll derivative and the application in organic solar cells**

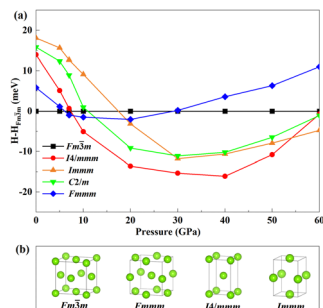
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Fengzhang Tang,\* Jiafei Pang,\* Jinni Yang, Xiaoyu Kuang\* and Aijie Mao\*

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**Structural evolution and superconductivity of thorium under high pressure and its modulation**

Lihui Zhan, Wenhao Fan, Junyi Miao, Shi He, Qingzhuo Duan, Xilong Dou and Cheng Lu\*

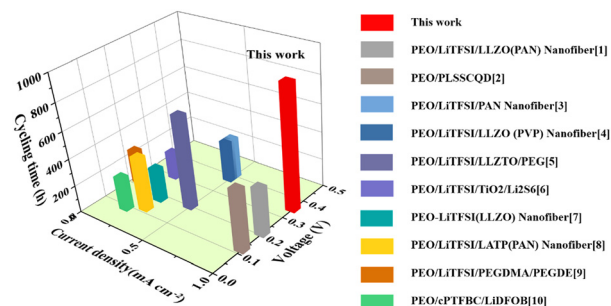


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# A strategy involving the use of 3D self-supporting B-N co-doped carbon nanofiber composite solid polymer electrolytes to stabilize the interface between polymer electrolytes and lithium metal

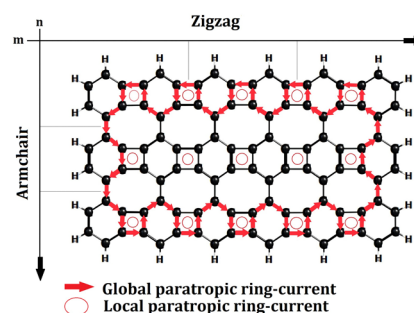
Yujie Wang,\* Lingling Sun, Xiaoli Li and Yan Zhang



25648

# Aromaticity of biphenylene networks

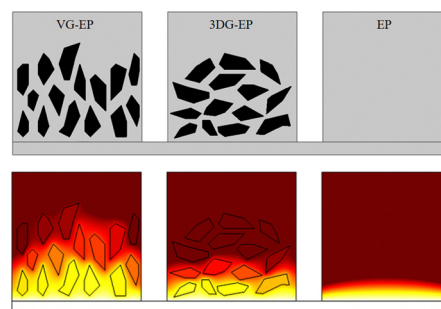
Lenara I. Valiulina,\* R. Valiyev, Victor N. Cherepanov and Elena V. Stepanova



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# Enhancing thermal transport of epoxy composites with vertically aligned graphene *in situ* grown on the thermal interface

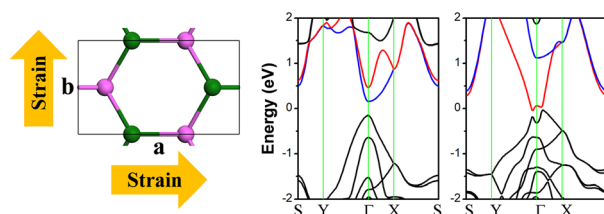
Jiaqiang Liao, Shijie Chen, Minjin Huang, Tao Rui, Zhi Qun Tian and Changzheng Li\*



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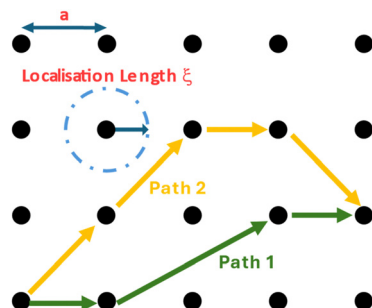
# Strain-tunable electronic anisotropy of the AlSb double-layer honeycomb structure

Hongsheng Liu,\* Yaning Li, Rui Chen, Yuanyuan Zhao and Junfeng Gao\*



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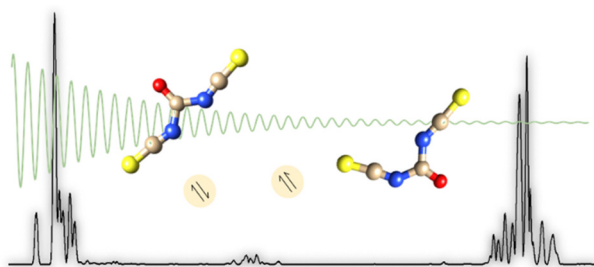
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## Theoretical analysis of electron transport in perovskite thin films

Ankur Bhaumik\* and Anshu Pandey

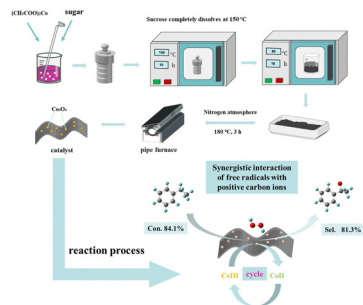
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## Rotational conformers and nuclear spin isomers of carbonyl diisothiocyanate

Eva Gougoula,\* Jonathan Pfeiffer, Melanie Schnell\* and Frank Tambornino\*

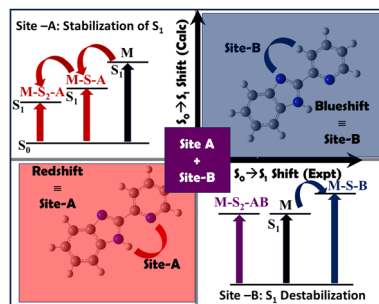
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## Green and efficient catalytic oxidation of ethylbenzene to acetophenone over cobalt oxide supported on a carbon material derived from sugar

Jinhong Li, Zhimei Song, Kaikai Cui, Haonan Li, Mei Han, Jing Wang and Lidong Chen\*

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Spectroscopic characterization of the complexes of 2-(2'-pyridyl)-benzimidazole and  $(\text{H}_2\text{O})_{1,2}$ ,  $(\text{CH}_3\text{OH})_{1,2}$ , and  $(\text{NH}_3)_{1,2}$  isolated in the gas phase

Arkaprabha Sen, Saurabh Khodia, Ramesh Jarupula, Simran Baweja, Bhavika Kalal and Surajit Maity\*

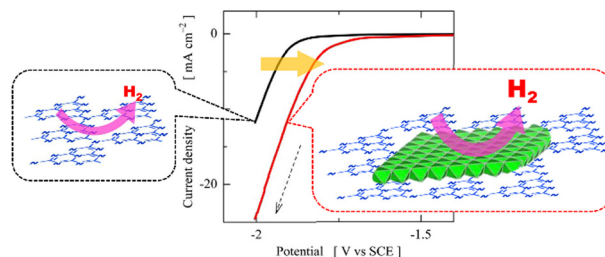


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### Enhanced electrocatalytic activity in hydrogen evolution reaction using 2D/2D nanohybrids of ruthenate nanoflakes and graphitic carbon nitride

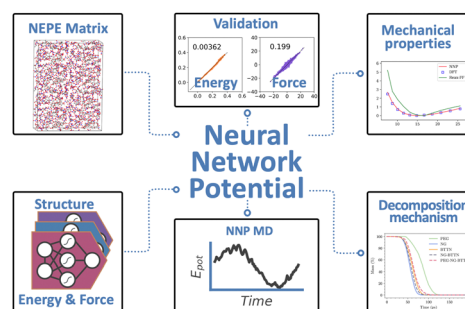
Takayuki Ban,\* Kazuki Inukai, Chika Takai-Yamashita and Kazuhiro Manseki



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### Uncovering the decomposition mechanism of nitrate ester plasticized polyether (NEPE): a neural network potential simulation

Mingjie Wen, Juntao Shi, Xiaoya Chang, Jiahe Han, Kehui Pang, Dongping Chen and Qingzhao Chu\*



## CORRECTION

25731

### Correction: Effects of BPQ binding on the nonadiabatic dynamics of excited electrons in poly(dG)–poly(dC) DNA under proton irradiation

Zhihua Hu, Zun-Yi Deng and Hong-Jian Feng\*

